Zero density limit extrapolation of the superfluid transition temperature in a unitary atomic Fermi gas on a lattice

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The superfluid transition temperature T_c of a unitary Fermi gas on a three-dimensional isotropic lattice with an attractive on-site interaction is investigated as a function of density n, from half filling down to 5.0×10^{-7} per unit cell, using a pairing fluctuation theory. We show that except at very low densities ($n^{1/3} < 0.2$), where T_c/E_F is linear in $n^{1/3}$, T_c/E_F exhibits significant higher order nonlinear dependence on $n^{1/3}$. Therefore, linear extrapolation using results at intermediate densities such as in typical quantum Monte Carlo simulations leads to a significant underestimate of the zero density limit of T_c/E_F. Our result, $T_c/E_F = 0.256$, at $n = 0$ is subject to reduction from particle-hole fluctuations and incoherent single particle self energy corrections.

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Experimental realization of superfluidity in cold atomic Fermi gases has given the BCS–Bose-Einstein condensation (BEC) crossover study a strong boost over the past decade. More importantly, main interests have been paid to the strongly interacting regime, where the s-wave scattering length a is large. In particular, the unitary limit, where the scattering length diverges, has become a test point for theories. As a consequence, the superfluid transition temperature T_c in a unitary Fermi gas has been under intensive investigation in recent years.

Apart from calculating T_c directly in the 3D continuum with various approximations [1–16], one important method is to calculate T_c on a lattice and then extrapolate to zero density. It has been argued that the zero density limit is identical to the continuum case. Indeed, this is the approach used by quantum Monte Carlo (QMC) simulations. For this approach to work, two conditions have to be met. First, the result obtained from the simulation at a given density has to be accurate; this requires that both the lattice size and the particle number have to be large enough. Second, the densities n at which the simulations are performed have to be in the asymptotic linear regime of T_c as a function of $n^{1/3}$.

It is extremely important to investigate this issue, because the results of QMC have often been taken with high credibility in the cold atom community, despite the large discrepancies between the results from different groups (as well as within the same group sometimes), and the small total fermion number and lattice size used. For example, using QMC, Troyer and coworkers [17, 18] reported $T_c/E_F = 0.152$, whereas Bulgac *et al.* [19, 20] reported $T_c/E_F = 0.23$ and 0.15 in different papers. Using the method of Ref. 17, Goulko and Wingate [21] found $T_c/E_F = 0.171$. Another recent result [22] from QMC gave $T_c/E_F = 0.245$. Although these different results do not seem to be converging, the above result of Troyer and coworkers [17, 18] has been widely cited and compared with recently. The simulations in Ref. 17 were done for lattice fermions at finite densities and then extrapolated to zero density. It is the purpose of the present paper to investigate how low in density one needs to go so that the simulations are in the asymptotic linear regime to ensure the accurateness of the zero density limit extrapolation.

In this paper, we will study the finite density effect on the zero density limit extrapolation by calculating T_c on a 3D isotropic lattice with an attractive on-site interaction, U, using a pairing fluctuation theory. This theory has been able to generate theoretical results in good agreement with experiment [12, 23]. To show how the lattice effect evolves with fermion density, we drop the complication of the particle-hole channel. Our result reveals that, as the density approaches zero, T_c/E_F does reach the 3D continuum value. However, linear extrapolation using data points calculated at intermediate densities, such as those in Ref. [17], will lead to a significant underestimate of T_c for the continuum limit. When particle-hole channel contributions are properly included [24], we expect that the zero density limit will yield $T_c/E_F = 0.217$, as directly calculated in the continuum.

Details of the pairing fluctuation theory can be found in Ref. 10 both in the continuum and on a lattice (see Ref. 24 for the treatment of the particle-hole channel effect). On a lattice, the fermion dispersion is give by $\xi_{\mathbf{k}} = 2t(3 - \cos k_x - \cos k_y - \cos k_z) - \mu \equiv \epsilon_{\mathbf{k}} - \mu$, where t is the hopping integral, $\epsilon_{\mathbf{k}}$ is the kinetic energy, and we have set the lattice constant a_0 to unity. We define Fermi energy for a given density n by the chemical potential for a non-interacting Fermi gas at zero T. In addition, a contact potential in the continuum now becomes an on-site attractive interaction U. Namely, we are now solving a negative U Hubbard model. The Lippmann-Schwinger relation reads $m/4\pi a\hbar^2 = 1/U + \sum_{\mathbf{k}}(1/\epsilon_{\mathbf{k}})$. Therefore, the critical coupling strength is given by $U_c = -1/\sum_{\mathbf{k}}(1/\epsilon_{\mathbf{k}}) = -7.91355t$. Here $m = t/2$ is the effective fermion mass in the dilute limit. In what follows, we shall set $k_B = \hbar = 1$.

To recapitulate our theory, the fermion self energy comes from two contributions, associated with the superfluid condensate and finite momentum pairs, respectively, given by $\Sigma(K) = \Sigma_{sc}(K) + \Sigma_{pg}(K)$, where $\Sigma_{sc}(K) = -\Delta_{sc}^2 G_0(-K)$ and $\Sigma_{pg}(K) = \sum_Q t_{pg}(Q) G_0(Q-K)$, with Δ_{sc} being the superfluid order parameter. $\Sigma_{sc}(K)$ vanishes at and above T_c. The finite momentum T-matrix $t_{pg}(Q) = U/[1+U\chi(Q)]$ derives from summation of ladder diagrams in the particle-particle channel, with pair momentum Q, where

the pair susceptibility $\chi(Q) = \sum_K G(K)G_0(Q-K)$ involves the feedback of the self energy via the full Green's function $G(K)$. As usual, we use a four vector notation, $K \equiv (i\omega_l, \mathbf{k})$, $Q \equiv (i\Omega_n, \mathbf{q})$, $\sum_K \equiv T\sum_l \sum_{\mathbf{k}}$, and $\sum_Q \equiv T\sum_n \sum_{\mathbf{q}}$, where ω_l (Ω_n) are the odd (even) Matsubara frequencies.

By the Thouless criterion, the T_c equation, given by $1 + U\chi(0) = 0$, now contains the self energy feedback. This is a major difference between our pairing fluctuation theory and those based on Noziéres and Schmitt-Rink (NSR) [1] or saddle point approximations [2].

After analytical continuation $i\Omega_n \to \Omega + i0^+$, one can Taylor expand the (inverse) T-matrix as $t_{pg}^{-1}(\Omega, \mathbf{q}) \approx Z(\Omega - \Omega_{\mathbf{q}} + \mu_{pair} + i\Gamma_{\mathbf{q}})$, and thus extract the pair dispersion $\Omega_{\mathbf{q}} = 2B(3 - \cos q_x - \cos q_y - \cos q_z)$. Here the imaginary part $\Gamma_{\mathbf{q}}$ can be neglected when pairs become (meta)stable [10].

At and below T_c, $\mu_{pair} = 0$ and $\Sigma_{pg}(K)$ can be approximated as $\Sigma_{pg}(K) = \Delta_{pg}^2/(i\omega_l + \xi_{\mathbf{k}}) + \delta\Sigma \approx -\Delta_{pg}^2 G_0(-K)$, with the pseudogap parameter Δ_{pg} defined as

$$\Delta_{pg}^2 \equiv -\sum_Q t_{pg}(Q) \approx Z^{-1} \sum_{\mathbf{q}} b(\Omega_{\mathbf{q}}) \,, \tag{1}$$

where $b(x)$ is the Bose distribution function.

Neglecting the incoherent term $\delta\Sigma$ in Σ_{pg}, we arrive at the total self energy $\Sigma(K)$ in the BCS form:

$$\Sigma(K) \approx -\Delta^2 G_0(-K), \tag{2}$$

where the total gap Δ is determined via $\Delta^2 = \Delta_{sc}^2 + \Delta_{pg}^2$. Therefore, the Green's function $G(K)$, the quasiparticle dispersion $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}$, and the gap (or T_c) equation all follow the BCS form, *except that the total gap Δ now contains both contributions from the order parameter Δ_{sc} and the pseudogap Δ_{pg}*. Thus the gap equation is given by

$$1 + U\sum_{\mathbf{k}} \frac{1 - 2f(E_{\mathbf{k}})}{2E_{\mathbf{k}}} = 0 \,, \tag{3}$$

where $f(x)$ is the Fermi distribution function. In addition, the number equation, $n = 2\sum_K G(K)$, is given by,

$$n = \sum_{\mathbf{k}} \left[1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \left[1 - 2f(E_{\mathbf{k}}) \right] \right] . \tag{4}$$

Equations (3), (4), and (1) form a closed set. For given interaction U, they can be used to solve self consistently for T_c as well as Δ and μ at T_c.

In Fig. 1 we plot T_c as a function of pairing strength $-U/6t$ for various densities from high to low. Here $6t$ is the half band width. For $n = 0.7$, the maximum T_c occurs on the BEC side of unitarity. Then it moves to the BCS side as n decreases. As n further decreases, the maximum moves slowly back to the unitary point. This should be contrasted with the 3D continuum case, for which the maximum occurs slightly on the BEC side. The fact that the maximum occurs on the BCS side manifests strong lattice effect at these intermediate densities; it is the lattice effect that causes difficulty for pair hopping and thus suppresses T_c. Even at density as low as $n = 0.005$, the maximum is still slightly on the BCS side.

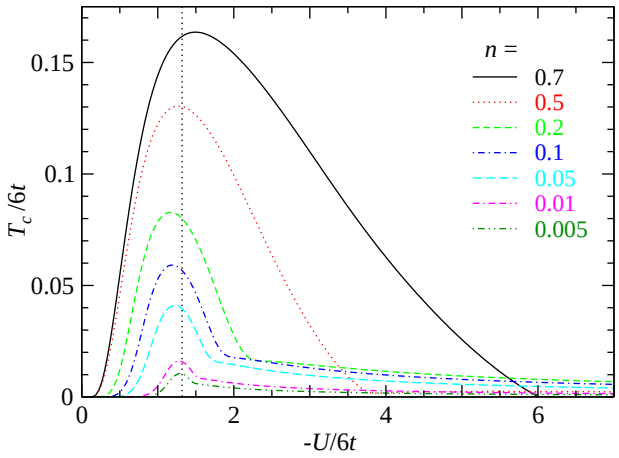

Figure 1. (Color online) Behavior of $T_c/6t$ as a function of the attractive on-site interaction $-U/6t$ on a 3D isotropic lattice for various density from high to low, as labeled. The unitary limit corresponds to $-U/6t = 1.31893$, as indicated by the vertical dotted line.

In order to compare with the continuum T_c curves (see Fig. 10 in Ref. 12 for example) more easily, we normalize the T_c curves by corresponding Fermi energy E_F, as shown in Fig. 2. For clarity, we have dropped the curves for the two high densities, $n = 0.7$ and 0.5. The lattice effect has made the peak around unitarity much more pronounced, and necessarily present in all different theoretical treatments of finite temperature BCS-BEC crossover [25]. As n decreases, this peak becomes narrower and moves closer to unitarity. Beyond the unitary limit, the curve for $n = 0.001$, as a low density example, exhibits a rapid falloff with pairing strength, and then decreases following the functional form $T_c \propto -t^2/U$. This is due to the virtue ionization during pair hopping in the BEC regime. At unitarity, a significant fraction of fermions form metastable pairs [10, 11] already at T_c, and thus they also see the lattice effect during pair hopping through virtue ionization. This suggests that the lattice effect will never go away in the unitary limit no matter how low the density may be. Figure 2 also reveals that, as n approaches zero, the maximum T_c/E_F as well as T_c/E_F at unitarity gradually increase.

Finally, presented in the main figure of Fig. 3 is T_c/E_F as a function of (cubic root of) density n in the unitary limit, down to $n = 5.0 \times 10^{-7}$, since the lattice effect is expected to vary as $n^{1/3}$ to the leading order, namely, $T_c(n)/E_F(n) = T_c(0)/E_F(0) - \alpha a_0 n^{1/3} + o(a_0^2/n^{2/3})$, α is a proportionality coefficient. Note that $a_0 n^{1/3}$ represents the ratio between the lattice period and the mean interparticle distance. At the same time, T_c/E_F and $T_c/6t$ are plotted as a function of n in the upper inset. It shows T_c/E_F increases rapidly near the very end of $n = 0$. The behavior of $E_F/6t$ is shown in the lower inset, in a log-log plot. In units of $6t$, both E_F and T_c vanish at $n = 0$ and reach a maximum at half filling [26]. In particular, $E_F = 6t$ at half filling, as expected.

Our result reveals that as n decreases from half filling, T_c/E_F decreases and reaches a minimum of 0.172 around

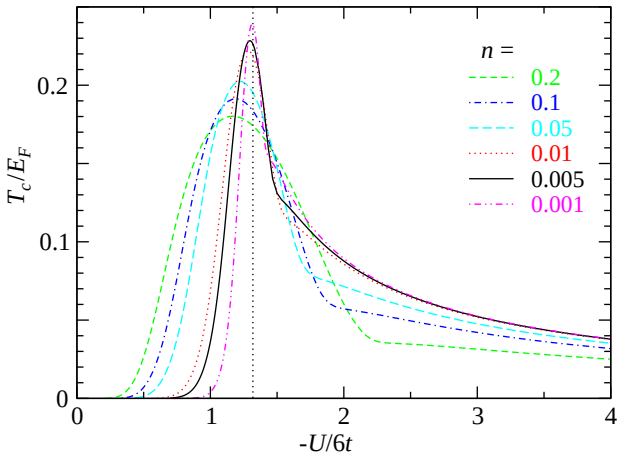

Figure 2. (Color online) T_c/E_F as a function of $-U/6t$ on a 3D isotropic lattice for various density from $n = 0.2$ to 0.005. The unitary limit corresponds to $-U/6t = 1.31893$, as indicated by the vertical dotted line.

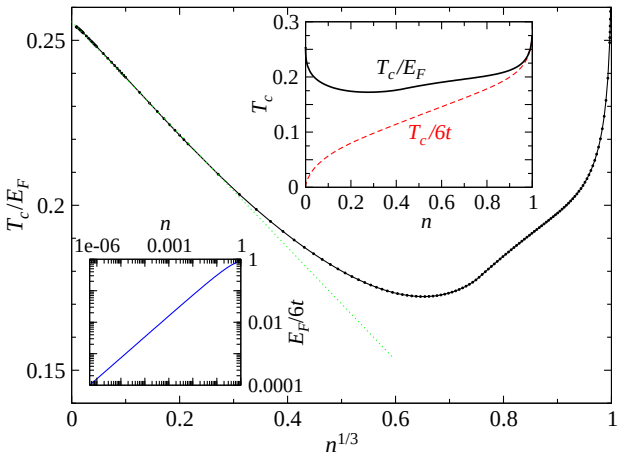

Figure 3. (Color online) T_c/E_F as a function of $n^{1/3}$ on a 3D isotropic lattice at unitarity. Shown in the lower left inset is $E_F/6t$ as a function of n, and plotted in the upper inset are T_c/E_F (black solid curve) and $T_c/6t$ (red dashed line) as a function of n. The (green dotted) linear extrapolation line obtained from fitting using data points below $n^{1/3} = 0.2$ yields $T_c/E_F = 0.2557$ at $n = 0$.

$n = 0.28$, and then starts to recover slowly. It does not accelerate until the very end of $n = 0$. The main plot suggests that T_c/E_F eventually does recover its continuum counterpart value, 0.256, but the curve exhibits a good linearity only for $n^{1/3} < 0.2$, i.e. $n < 0.008$. At $n = 5.0 \times 10^{-7}$, we finds $T_c/E_F = 0.254$, close to 0.256. Using the data below $n^{1/3} = 0.2$, our extrapolation (the green dotted line) leads to $T_c/E_F = 0.2557 \approx 0.256$ for the continuum limit. Note that the data points for $n^{1/3} > 0.3$ shows a rather obvious deviation from the lower n extrapolation line. This implies that the range of density for extrapolation used in Ref. 17 is still far from the asymptotic linear regime. In fact, $n^{1/3} > 0.3$ cannot be regarded as $\ll 1$. Indeed, the recent result of Goulko and Wingate [21] seems to confirm this point. They pushed their simulations down to $n^{1/3} \approx 0.23$ (albeit with a big error bar), and obtained $T_c/E_F = 0.173$ for the zero density limit using a linear extrapolation. One can also see from their Fig. 7 that, without this lower density data point, they would have obtained a lower value for T_c/E_F. In addition, their quadratic fit would yield $T_c/E_F \approx 0.19$. Finally, we note that a closer look of Fig. 3 of Ref. 17 suggests that the lowest density point (also with a big error bar) actually already shows that their curve starts to bend upward, away from the straight extrapolation line. Although not conclusive, this observation agrees with the T_c/E_F curve in Fig. 3.

Despite the big difference between our theory and the QMC approach, it is reasonable to expect that the lattice effect has a rather similar effect on T_c/E_F. Therefore, we believe that in order to obtain an accurate value of T_c/E_F in the zero density limit using a linear extrapolation, one needs to perform QMC down to $n^{1/3} \sim 0.1$ (i.e. $n \sim 1.0 \times 10^{-3}$) or lower.

A later paper by Troyer *et al.* [18] claimed that they confirmed their lattice fermion result by working in the continuum limit. However, it is likely that the lattice effect was actually introduced back through their Eqs. (3) and (4) and the periodic boundary condition [27]. Indeed, this has been confirmed by Ref. [28], which was partly motivated by the preprint [29] of the current paper. Furthermore, the thermodynamic limit value was obtained from a linear fit of *only 3 data points*! In this later paper, they performed simulations at unitarity down to $n \approx 0.05$ (with $l_0 = 1$), or $n^{1/3} = 0.37$. Unfortunately, this density was still far from low enough to enable an accurate extrapolation. Above this density, the curve in the main figure of Fig. 3 shows significant deviation from linearity, caused by contributions of order $n^{2/3}$ and higher. Our result shows that the densities used for the QMC simulations in Ref. [17] were not low enough to ensure a good linear zero density limit extrapolation of T_c/E_F as a function of $n^{1/3}$.

The QMC simulations by Bulgac *et al.* were also done on a lattice, and the number of atoms and the lattice sizes were too small (e.g. only 50-55 atoms on an 8^3 lattice in Refs. 19 and 20, equivalent to $n = 0.1 \sim 0.11$ or $n^{1/3} = 0.46 \sim 0.48$) to study the dilute limit as we have done here. In the context of dynamical mean field theory, Privitera et al [30] studied the importance of nonuniversal finite-density corrections to the unitary limit and found that "densities around $n \simeq 0.05 - 0.01$ are not representative of the dilute regime".

It should be noted that our E_F is the actual Fermi energy in the 3D lattice, whereas Troyer and coworkers [17] simply defined $E_F = tk_F^2 = t(3\pi n)^{2/3}$. This definition will become the true Fermi energy only in the dilute limit.

Finally, it is interesting to note that on the lattice, the interaction at unitarity, U_c, is density independent so that U_c/E_F will scale to infinity as n approaches 0. In contrast, in the continuum, a contact potential can be regarded as the cutoff momentum $k_0 \to \infty$ limit of an s-wave interaction, $U(k) = U\theta(k_0 - k)$, which has $U_c = -2\pi^2/mk_0$. Apparently, this U_c is scaled down to 0 for a contact potential. This dramatic contrast for U_c between 3D lattice and 3D continuum seems to suggest that the 3D continuum cannot be simply taken as the zero density limit of a 3D lattice. Indeed, the fermions are always subject to the lattice periodicity no matter

how low the density is.

Without including the self energy feedback in the T_c equation [11], the NSR theory [1, 4, 31] and the saddle point approxmation [2] predicted $T_c/E_F = 0.22$. Other approaches reported $T_c/E_F \approx 0.26$ [3], 0.15 [5], and 0.16 [6], the last of which exhibits *unphysical* non-monotonic first-order-like behavior in entropy $S(T)$. Floerchinger *et al.* [7] found $T_c/E_F = 0.264$ even after including particle-hole fluctuations. Within the present theory, we reported $T_c/E_F = 0.256$ [10–12].

Experimentally, the Duke group [32], in collaboration with Chen *et al.*, found $T_c/E_F = 0.27$ through a thermodynamic measurement in a unitary ^{6}Li gas. Later, they [33, 34] obtained 0.29 and 0.21 by fitting entropy and specific heat data with different formulas. The latter value was obtained assuming a specific heat jump at T_c, which may not be justified in the presence of a strong pseudogap at T_c (See, e.g., Refs. 12, 35, and 36). According to our calculations, T_c at unitarity in the trap is only slightly higher than its homogeneous counterpart, 0.272 versus 0.256. Similar small difference in T_c between trap and homogeneous cases is expected from other theories as well. Therefore, these measurements imply that the homogeneous T_c/E_F is about $0.25 \sim 0.19$. Recently, Ku *et al.* [37] reported $T_c/E_F \approx 0.167$ for a homogeneous Fermi gas by identifying the lambda-like transition temperature.

Our result demonstrates that the $n \to 0$ limit of the lattice T_c/E_F does approach that calculated directly in the continuum. We expect this to remain true when the particle-hole channel contributions are properly included. In that case, we obtain $T_c/E_F = 0.217$ at unitarity [24], consistent with some of the above experimental measurements. Finally, we note that inclusion of the incoherent self energy $\delta\Sigma$ in our calculations would further reduce the value of T_c/E_F [24], bringing it closer to the result of Ku *et al.* [37].

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